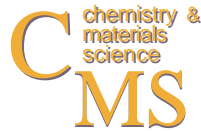
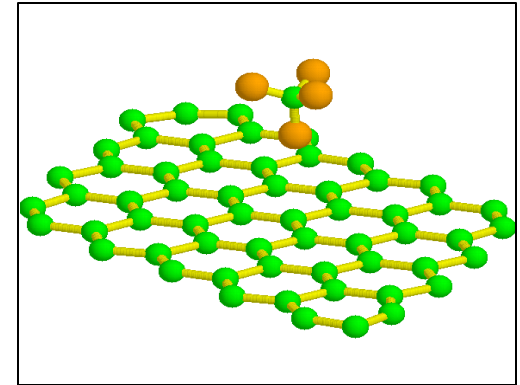
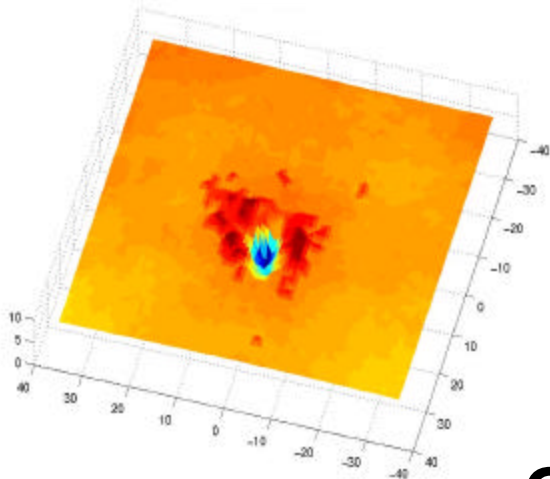


Atomistic simulations in fusion energy science



E.M. Bringa
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**PFC meeting
Oakbrook, November 2003**

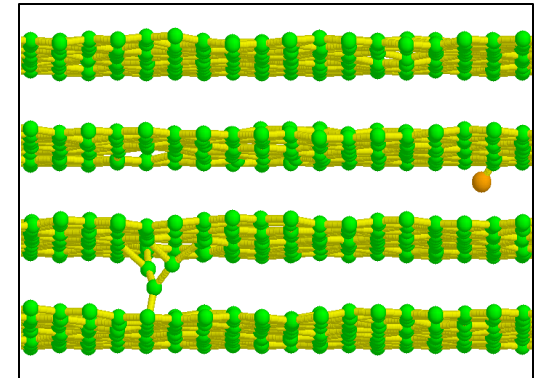


with contributions from:

A. Caro, G. Gilmer (LLNL),
B.D. Wirth (UC Berkeley)

Collaborators:

T. Rognlien (LLNL), J.P. Allain (ANL), S.
Stuart (Clemson), S. Zybin (Georgetown)



Outline



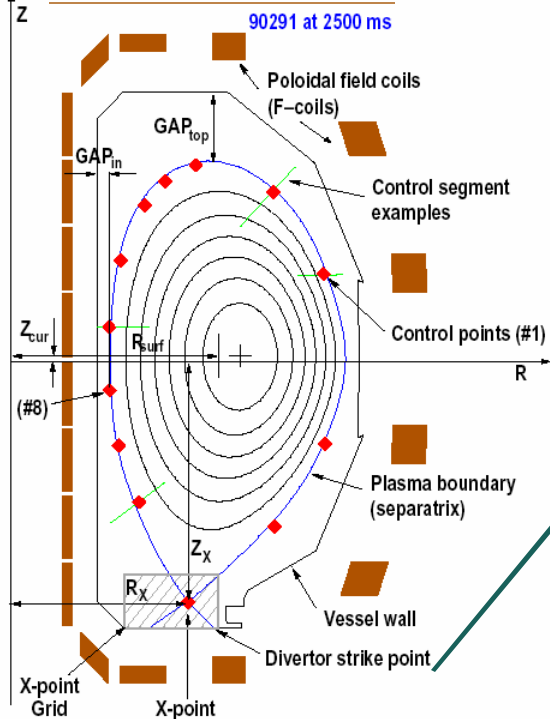
- **Why do we need atomistic simulations in PFC?**
- **What can we do in PWI (Plasma Wall interaction)?: near and long term plans at LLNL**
- **Details on Kinetic Monte Carlo (KMC)**
- **Can we integrate atomistic codes with kinetic plasma codes?**
- **Details on MD potentials upgrade**
- **Summary**

Plasma Wall Interactions

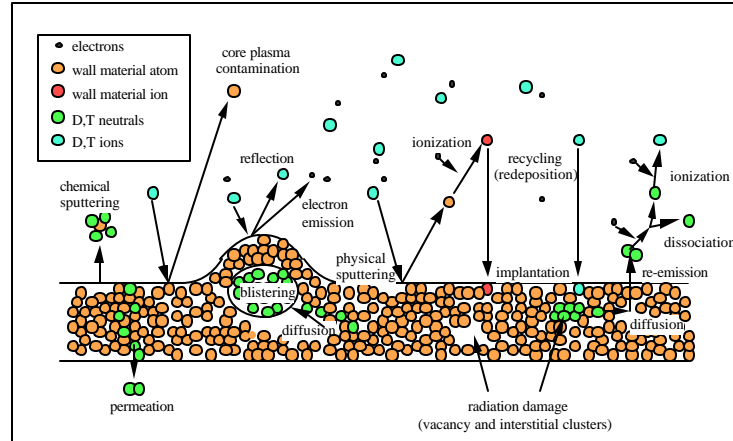


- Plasma impurity content is very important to machine operation through the pedestal. Predictive models require improved input & modeling interfaces for boundary processes that control hydrocarbon contamination of the plasma, resulting from surface erosion by chemical and physical sputtering

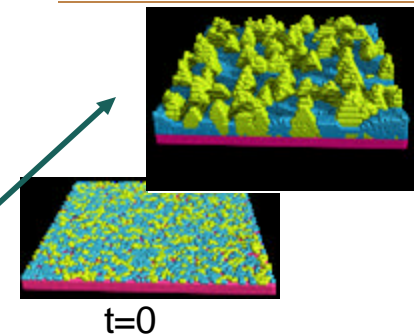
Plasma x-section



Divertor surface physics



Surface evolution



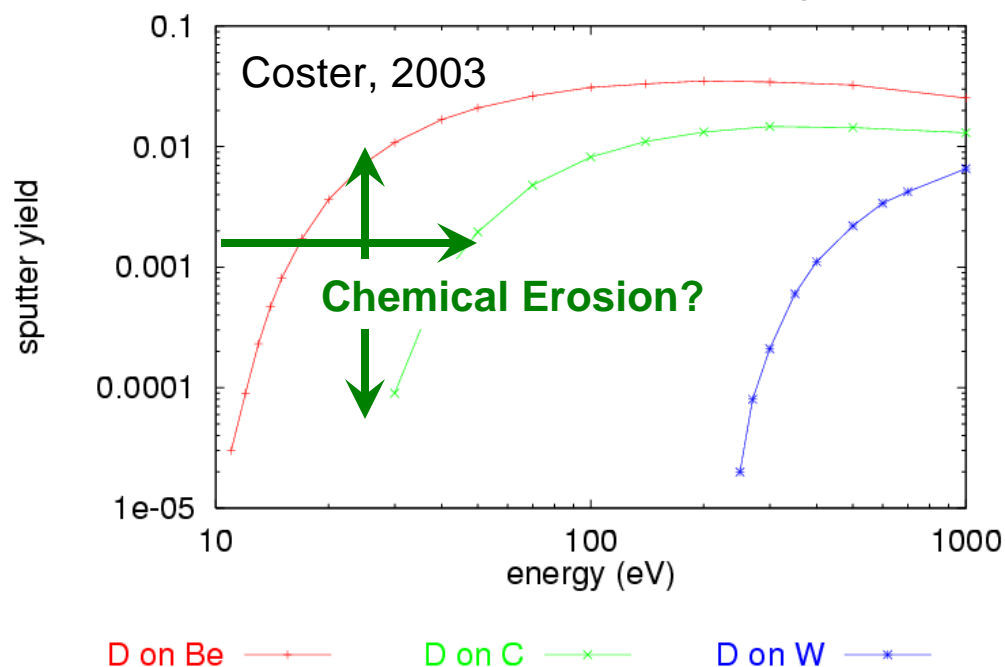
Surface physics and molecular processes control plasma-divertor interaction, and correspondingly erosion and re-deposition that is mediated by ion reflection, chemical and physical sputtering → all of these processes influence the topological and chemical evolution of the surface, further impacts erosion and plasma contamination

Impurities affect the edge-plasma power balance



- Sputtering at walls is main source of impurity contamination
- Sputtering depends on plasma and wall dynamic conditions

MODEL PHYSICAL SPUTTERING (wrong at low E)



Impurities in tokamaks: 30-70% of radiative power mostly in the edge.

Current models (e.g., UEDGE, WBC) rely on 'static' tabulated rates for sputtering yields (no flux/surface dependence).

ITER divertor will operate with low energy incident ion/neutral < 200 eV

- Sputtering at low energies is dominated by chemical sputtering
- Chemical sputtering experiments are difficult at low energies →
- Uncertainties in impurity contamination generation are > 2 orders of magnitude

ELM's regime: 200 eV- few keV particle bombardment and erosion, often not included in current plasma codes

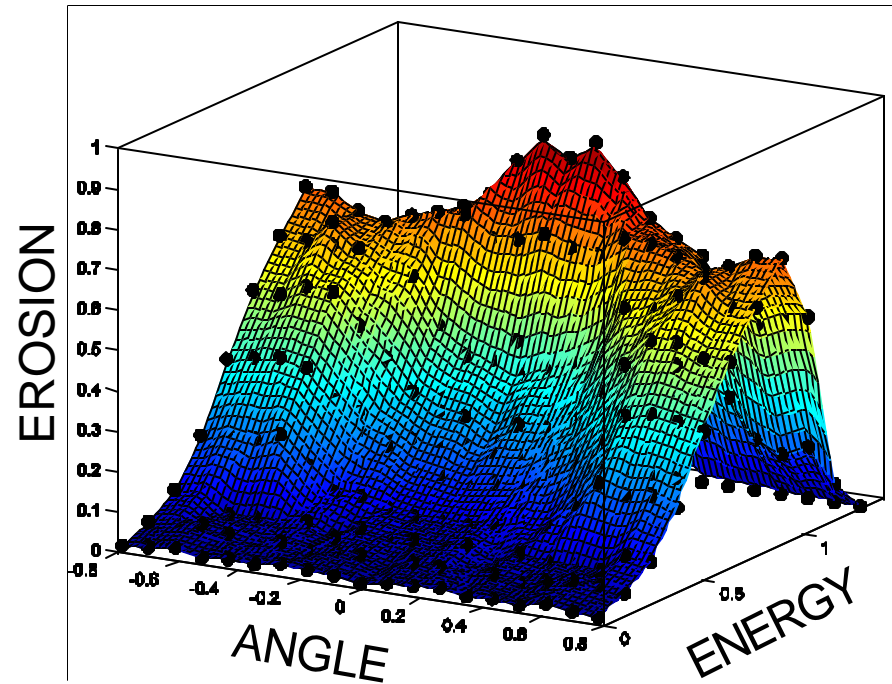
Plasma-surface modeling: near-term (1-2 year) objectives



Uncertainty to be resolved: Sputtering for multiple plasma/wall conditions

Multi-dimensional (ion/neutral type, incident energy, angle, flux, surface temperature and chemical/spatial topology) sputtering yield tables for near-surface kinetic and fluid whole-edge transport codes

Large number $O(10^5-10^6)$ of MD simulations required. LLNL has unique experience and high performance computing capability.



Coupling between plasma-surface - sheath - turbulent edge models important for physically-reliable simulations.

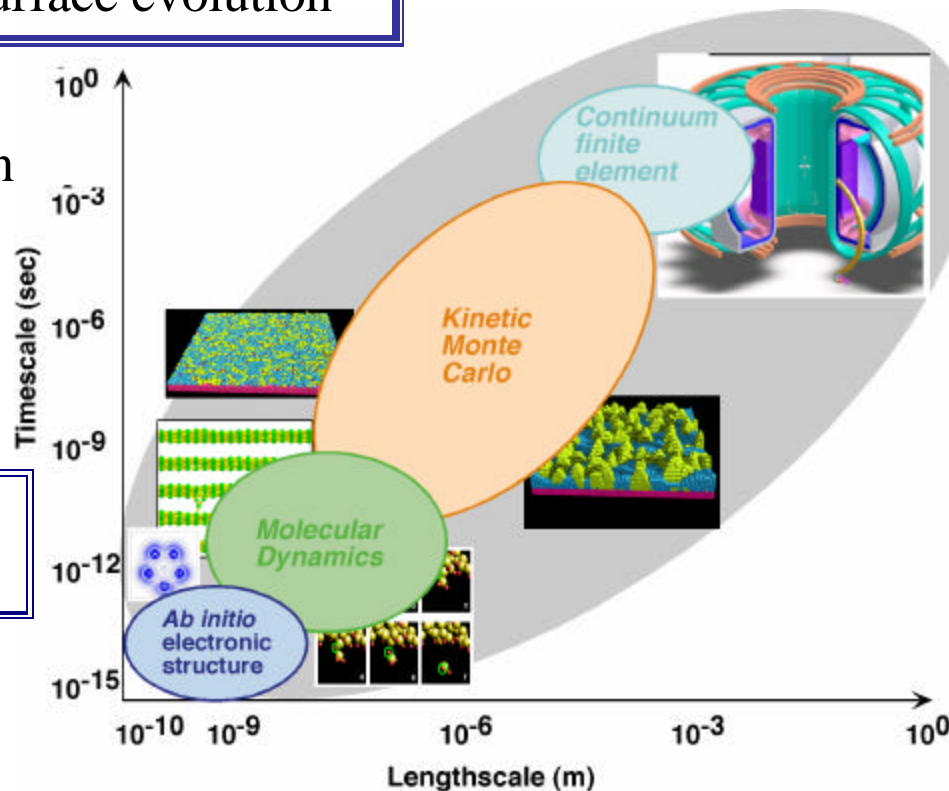
Plasma-surface modeling: longer-term (2-3 year) objectives



Uncertainty to be resolved: dynamic surface evolution

Develop kinetic Monte Carlo that would dynamically obtain surface evolution (ion bombardment, impurity contamination, Chemistry and topology) and communicate with plasma edge/sheath physics codes.

Modeling methodology appropriate for simulating tritium transport & retention.



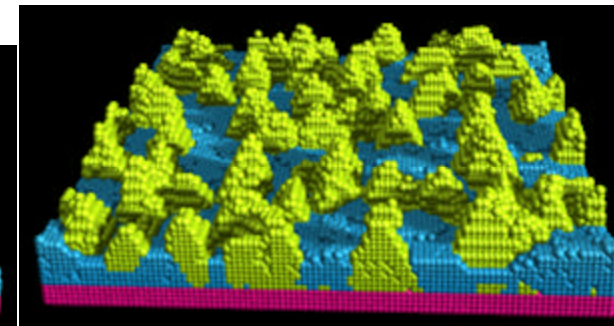
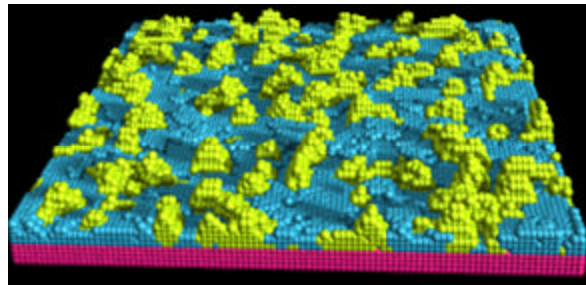
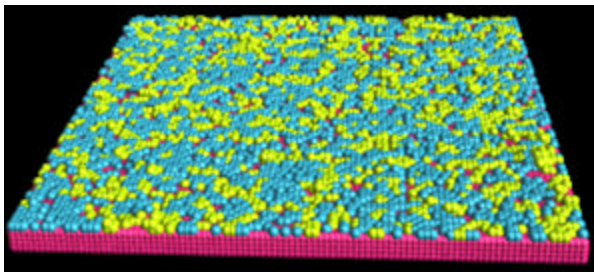
The outcome of this work is:

- Accurate predictions of impurity contamination as (dynamic) boundary conditions for plasma edge/sheath physics codes.
- Spin-off: tritium retention mitigation strategies as a result of physically-based simulations of tritium inventory.

ON-LATTICE KINETIC MONTE CARLO MODELS



- Impinging ions/atoms follow ballistic trajectories, impinge, diffuse.
- Monte Carlo events are assigned rate constants:
 1. Impingement rates for ions/atoms: k_i (function of energy)
 2. Diffusion hop rates: v_j
 3. Time step $\Delta t \propto 1 / [\sum k_i + \sum v_j]$
- Lattice model of atomic positions in crystalline grains.
- Efficient code: bookkeeping lists of all atoms in near-surface region allow events to be picked with probabilities proportional to rate constants.
- Potential for atomic interactions derived from MD configuration energies and saddle points.



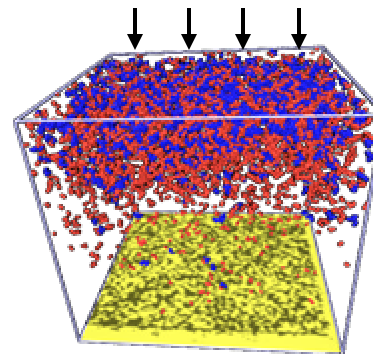


MC simulation of implantation of 5keV Si ions, $10^{14}/\text{cm}^2$, and an anneal at 800°C. Interstitials cluster into {311} defects.

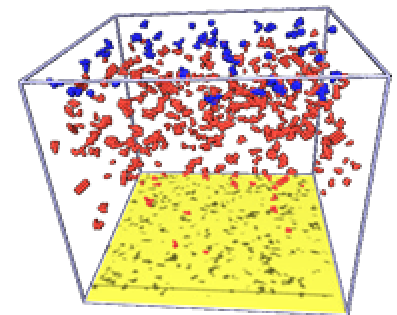
Diaz de la Rubia & Gilmer, G. H., Nature Materials **1**, 89, (2003). Law, Gilmer, Jaraiz, MRS Bulletin, June 2000, p. 45

Monte Carlo Events:

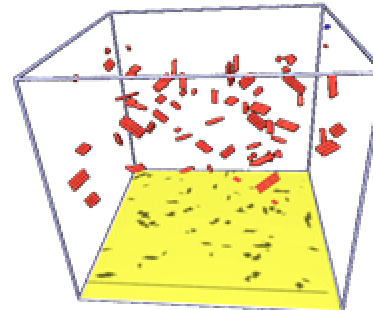
- Ion implantation and damage (MD and MARLOWE binary collision code).
- Point defect diffusion and recombination.
- Impurity/point defect binding and diffusion.
- Clustering of point defects and impurities.
- Recombination of point defects at free surface.



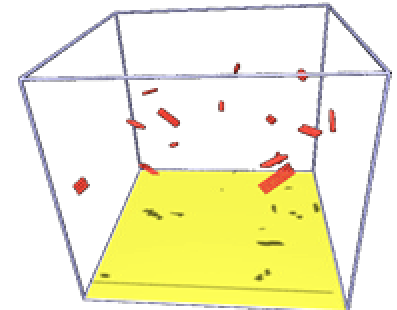
Initial damage



Anneal, $t = 1$ sec



$t = 40$ sec



$t = 250$ sec

Interstitials red, vacancies blue.

Interstitial $\langle 311 \rangle$ clusters are formed.



How much does classical MD cost?



N_{steps} = number of time steps; N = total number of atoms,
 R_{cut} = cut-off radius of potential, N_{cut} = number of atoms within radius R_{cut} ,
 F = cost of evaluating forces for a given atom
potential dependent: if $F_{\text{pair}}=1 \rightarrow F_{\text{EAM}} \sim 3, F_{\text{REBO}} \sim 20, F_{\text{AIREBO}} \sim 1000$

$$\text{COST} \propto F N_{\text{steps}} N_{\text{cut}} f(N) \propto F N_{\text{steps}} (R_{\text{cut}})^3 f(N)$$

Serial codes:

No neighbor list $\rightarrow f(N) \propto N^2$ (Only practical for $N < 2,000-5,000$)

Neighbor list $\rightarrow f(N) \propto N$

pair potential \rightarrow memory limited: neighbor list 1 GB RAM for $N \sim 500,000$

many-body potentials $\rightarrow F$ very costly \rightarrow practical for $N < 5,000-30,000$ atoms

N large/ F costly \rightarrow need parallel code

Parallel Codes:

Domain decomposition $\rightarrow f(N) \propto N$

PRICE: communication overhead \rightarrow impractical if $N/\text{CPU} < 2,000-5,000$

MDCASK (LLNL): evaluation of $F \sim 80\%$, communication $\sim 15\%$, various $\sim 5\%$.

On-the-fly MD in plasma code?



(All estimates for 64 CPU's unless noted otherwise)

How much does it cost to run an MD code using (REBO I +long range) potentials?

1 single calculation (1 ps, 5 nm³) → 0.5 hours

1 point of the sputtering surface → ~10³-10⁴ single calculations → ~3 weeks

Full sputtering surface → ~10³ points → 3000 weeks

(~60 years, but 3 years if using 1280 CPU's all the time).

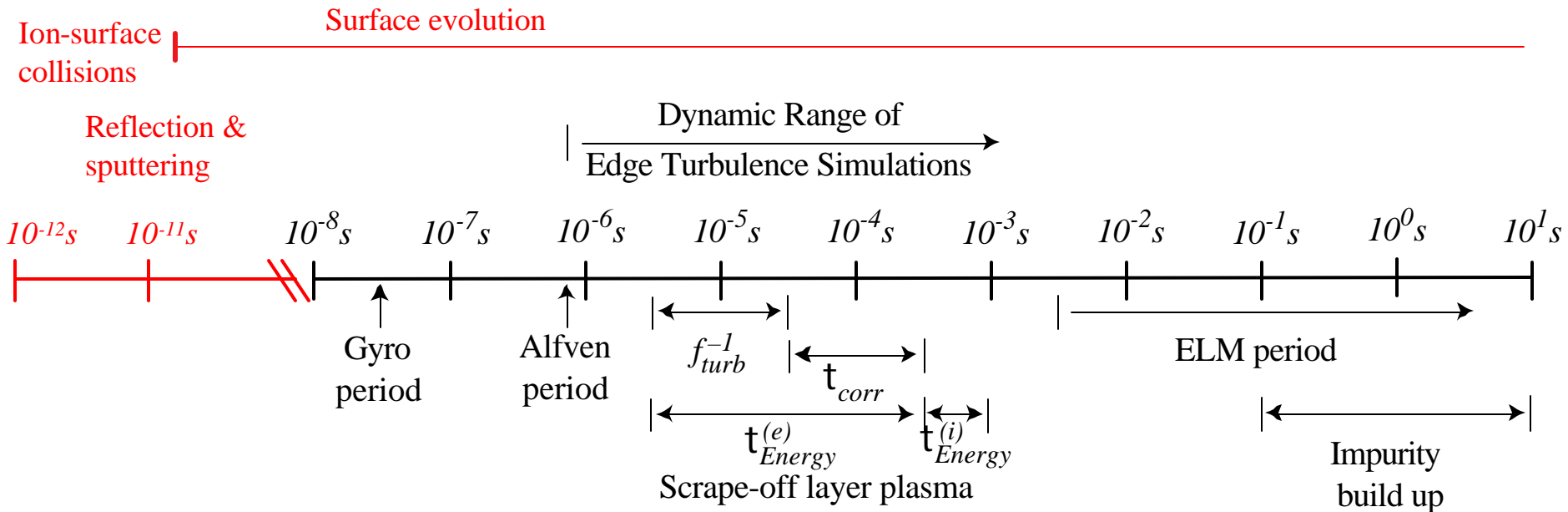
How much does it cost to run a hydro code? 10 ms → 0.5 hours

How much does it cost to run a kinetic code?

(BOUT3D, 1ms): ~1 week; (LLNLcode-5D, 1 ms) → ~100 weeks (~2 years)

MD cost ≥ cost of 5D turbulent plasma code →
sputtering surface: (coarse MD) + (MD-informed models)

Wide Range of Time Scales Challenges Computational Resources



If we want to do concurrent plasma+WBC+KMC+MD code, what can we do?

Possible solution:

- 1- Coarse-grained sputtering tables from MD, and use that to feed plasma codes (WBC+UEDGE, etc)
- 2- Run plasma code concurrently with KMC-surface evolution code. Feedback between them provides consistency.
- 3- Periodically, devote a chunk of CPU's to run few cumulative MD simulations using evolved KMC surface as the initial condition. Use result as new input for KMC and plasma code.

How do we get started with MD of hydrocarbons?



Need good reactive empirical (fast) potentials → “chemistry”

REBO I (Reactive-Empirical-Bond-Order, $R_{\text{cut}}=2 \text{ \AA}$)

Brenner *et al.* 1990-1992. Bond-order term has 3-body contributions. No dispersion forces (long range), no repulsion/attraction term for non-bonded atoms → Graphite planes not bonded (distance between planes $\sim 3.3 \text{ \AA}$).

REBO I + (dispersion/non-bonded), $R_{\text{cut}} \sim 10 \text{ \AA}$

Various implementations. MDCASK (LLNL): *parallel implementation (A. Kubota)*!

REBO II, $R_{\text{cut}}=2 \text{ \AA}$

Brenner *et al.* 2002. Re-parametrization of Brenner I, including new functional forms

AIREBO (Adaptative-Intermolecular REBO, $R_{\text{cut}}=10 \text{ \AA}$)

Stuart *et al.*, 2000-2003: REBO I + LJ-(bond-order) + torsion (4-body)

Tight-Binding based BOP ($R_{\text{cut}}=2.4 \text{ \AA}$)

Pettifor+Oleinik (1999-2003): new version has both 3 and 4 body terms. SLOW

ReaxFF [REActive Force Field, $R_{\text{cut}}=3.9 \text{ (LJ)}$ - $\infty \text{ (Coulomb)}$]

Van Duin *et al.* (2001-2003): BOP+LJ+torsion+Coulomb. VERY SLOW, but available for several species (H,C,O,N, Si, Al,...)

What are bond-order potentials?



One route is through a **MANY-BODY EXPANSION:**

$$U = \underbrace{\sum V^{2B}(R_i, R_j)}_{\text{two-body}} + \underbrace{\sum V^{3B}(R_i, R_j, R_k)}_{\text{three-body}} + \underbrace{\sum V^{4B}(R_i, R_j, R_k, R_l)}_{\text{four-body}} + \dots$$

higher order

They are a way to improve on two-body interactions

Assume potential energy can be expanded in terms of bond stretches and angle bends:

$$U = \underbrace{\sum \text{bond stretch}}_{\text{two-body}} + \underbrace{\sum \text{angle bend}}_{\text{three-body}} + \underbrace{\sum \text{stretch-bend}}_{\text{three + higher}} + \underbrace{\sum \text{stretch-stretch}}_{\text{three-body}} + \underbrace{\sum \text{bend-bend}}_{\text{four + higher}} + \dots$$

The energy is written in a form similar to a pair potential but with a many-body bond-order function that modulates the attractive pair term:

$$U_{\text{atom}} = \sum_{ij} [A e^{-a r_{ij}} - b e^{b r_{ij}}]; \quad U_{\text{tot}} = \sum U_{\text{atom}}$$

b: many-body bond-order function

Adapted from D. Brenner's web site

<http://www.mse.ncsu.edu/CompMatSci/Tutorial/listing.html>

What can AIREBO do better than REBO?



(besides graphite planes being bonded!)

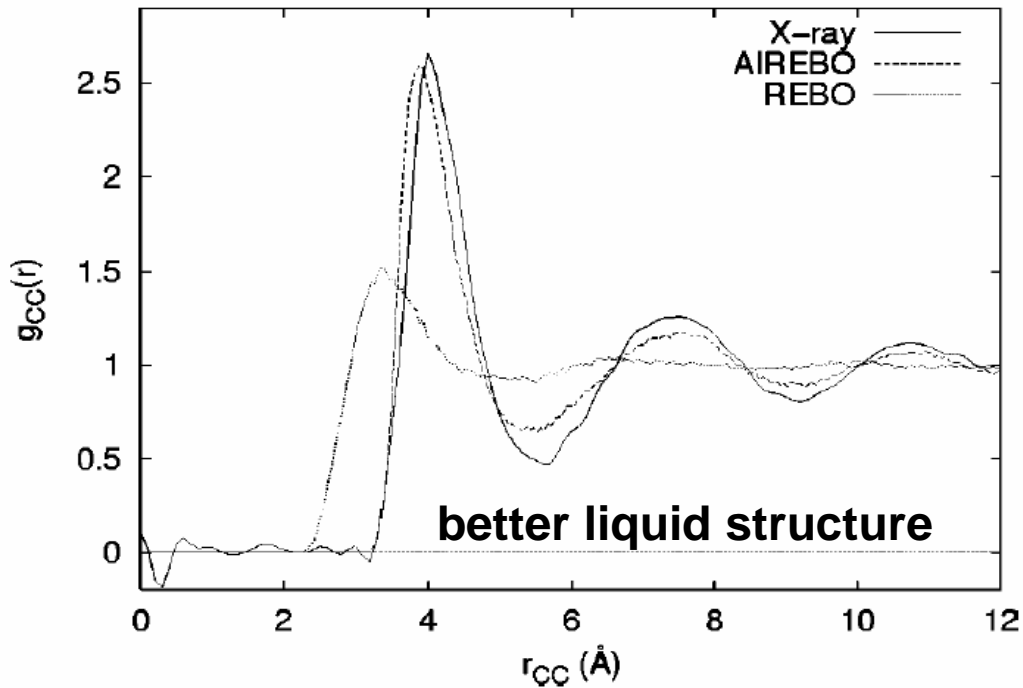
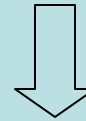


FIG. 2. Carbon-carbon pair correlation function $g_{CC}(r)$ for liquid methane at 92 K. Curves represent results from x-ray diffraction (Ref. 48), the AIREBO model, and the REBO model.

Stuart *et al*, J. Chem. Physics **112** (2000) 6472

Better description of radicals than REBO

REBO+ torsion + dispersion
(LJ)+nonbonded repulsion via
an adaptive method



suitable for studying reactivity
in molecular condensed
phases.

Overcomes the limitations of the
REBO potential in studying systems
with intermolecular interactions.

It has been designed for molecular
systems such as liquid hydrocarbons
(specially alkane liquids), thin films,
and small hydrocarbon molecules

What can we do with AIREBO at LLNL?

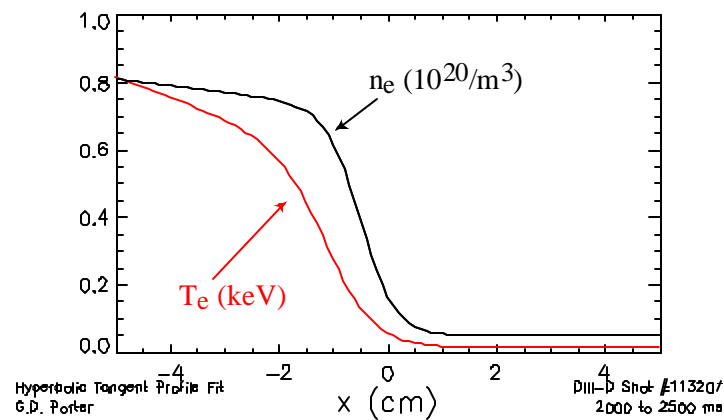


- Source code already obtained directly from the author (S. Stuart, Clemson University) as part of his MD package.
- Code is serial and ~50 times slower than REBO I
- Need to add some capabilities to do ion bombardment)
- Serial version can be used to generate relaxed samples (graphite+aC:H), that can be used as initial condition for further studies.
- Calculate sputtering yield for one energy and compare to REBO I results (Salonen *et al*, Allain *et al*, etc.), eg. 10 eV D → graphite.
- **Implement parallel version of AIREBO. Collaboration with S. Zybin (Georgetown University).**

Summary: PWI needs multiscale materials approach

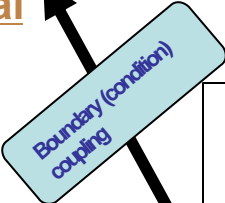


- Couple plasma edge models with physically-based multiscale materials models.
 - Predict hydrocarbon sputtering, erosion, re-deposition/re-sputtering
- ⇒ Surface evolution and feedback on plasma edge/H-mode pedestal
 - physically based material simulations
- ⇒ **Reliable estimates of tritium inventory**, can guide tritium mitigation strategies

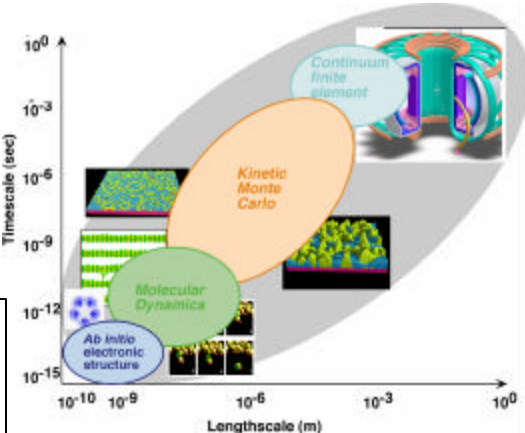
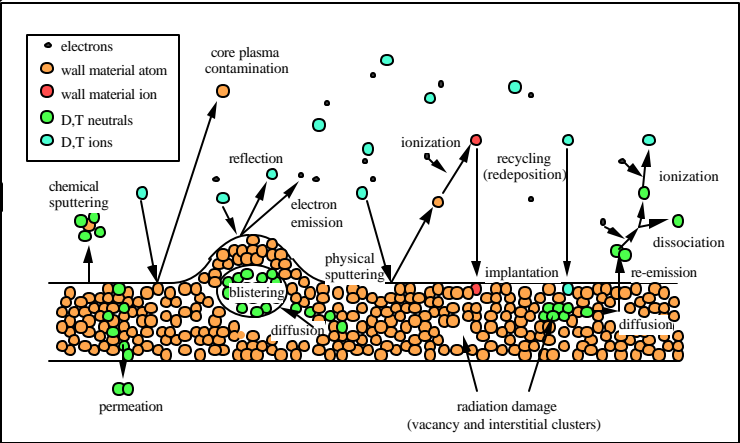


Plasma edge/pedestal physics & chemistry models

- VFTRIM
- REDEP
- HEIGHTS
- BPHI-3D
- UEDGE-2D



Divertor surface evolution models



- VASP
- MDCASK
- BIGMAC
- MICRO3D
- FEM